Introduction to Materials Science and Engineering
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Lecture – 20
ABCABC stacking of close-packed spheres

Hello. So, we have been talking about a close packing of equal size disphere and in particular we looked at one stacking sequence the A B A B stacking sequence in detail in the last video and we analyzed it is structure in terms of lattice and motive. Now the time has come to look at the other sequence which we said is also quite common in structure of crystals and that is the ABCABC stacking of spheres.

So, we will do the same we will try to analyze this structure in terms of lattice and motive.

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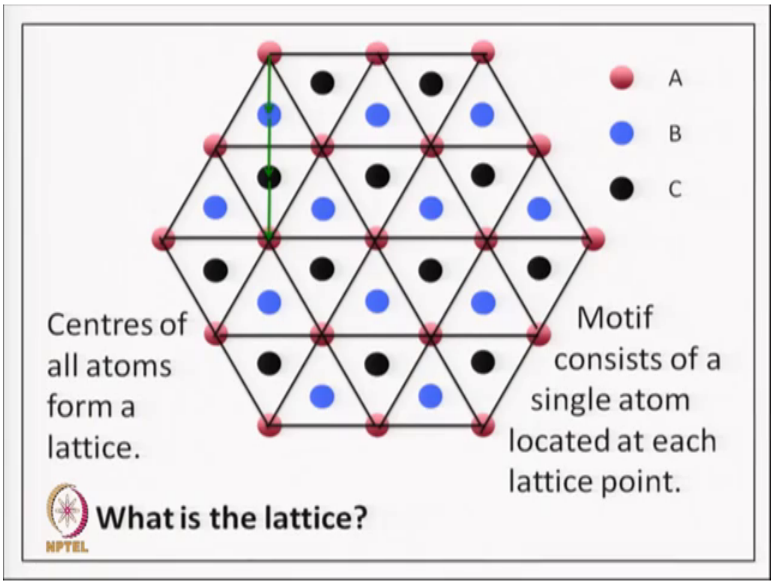

So, let us look at let us begin with our close packed structure you can see that each sphere it is surrounded by 6 spheres. So, this is a single 2 dimensional closed pack layer. When we start putting the next layer about this we get a stacking sequence and as we have seen while discussing hexagonal close packed structure, that there are 2 different kinds of locations where the next layer atoms can be put.

I can put the next layer atom either. So, the these are the a layer we will say in terms of our stacking designation and we can put the next layer represented by this blue sphere on a triangle of 3 atoms, triangle of 3 red atoms below and these 3 atoms are forming a triangle which is pointing upward. Such sites we will call the B side. So, this blue atom is representing A B atom note that I am using B is the blue color, but chemically these are supposed to be same element.

So, they are of the same chemical nature. Now if I place atoms at all of such triangles which are pointing that I get the next layer the B layer a still the third site is available which is the C side. So, my third layer in the hexagonal close pack layer is tracking sequence we stack the third layer exactly above A. So, we got A B A, but that was one possible option another option is still open to us that to put the third layer not exactly above A, but on these sites which have not yet been used.

So, those are the C sides. So, the centroid of a triangle which is pointing down it defines the location of C side and if I put my third layer on these side then that is the C layer. So, if I fill all the sides I get exactly identical close packed layer, but shifted at the third layer. And then if I continue the sequence ABC ABC then I get a crystal structure which we now wish to analyze in terms of lattice and motif.

To analyze it to find the lattice of this structure we have to look at whether one important question is whether all atoms are identical in the lattice sense or not. Recall that in hexagonal close packed structure A B A B stacking. Also, we had done this exercise and there to our surprise in a way we found that the a and B layer atoms are not equivalent in the lattice sense. So, the hcp crystal structure had 2 different kinds of atoms or 2 atoms in the motif.

We do the same exercise here. So, we start with a red sphere and we look we go in this direction that is centroid of this triangle. So, horizontally we go into the same plane as a red plane up to the centroid of the triangle and then we lift ourselves one inter planar is facing up to reach the B atom. Now the question is the B atom also having identical neighbor at the same vector displacement.

So, if we go by the same vector displacement we find that I travel exactly to the location which is called C and if I lift myself up I reach the C atom. So, this this C atom was missing in the hexagonal close packed structure that is what made A and B distinct because A had a neighbor B, but we did not have the neighbor C, but now in this current ABC stacking sequence we find that A has a neighbor B at this vector displacement B also has a neighbor C at the same vector displacement.

Of course, if we continue and find try to find the neighbor of C we find that the next a layer up there is A layer above C also because the stacking sequence is ABC ABC. So, the same vector displacement will take me from C also to an equivalent atom in E. This analysis of course, we have done it in only one direction you have to see all neighbors. So, you can repeat this analysis in other directions for other neighbors and once this is done it is found that all centers of all atoms are equivalent in the lattice sense and so they form a lattice.

So, this is a very, very important conclusion and this makes this ABC ABC stacking sequence very distinct from ABAB stacking sequence where all atoms were not forming a lattice and there was a 2-atom motif, but here since all atoms are forming a lattice we have a single atom motif. So, motif consists of a single atom and it is located at each lattice point all the points seen here are now lattice points, but what lattice the question is if all atoms are forming a lattice what is that lattice we are talking about because the lattice has to be 1 of the 14 bravais lattices.

So, that is the question which we now address and it turns out that this question for ABC ABC stacking is not a simple one. So, let us try to look at it little carefully. Recall that we are trying to stack 2-dimensional hexagonal layer. So, hexagonal symmetry is already inherent in the layer itself. So, the fact that by AB AB is stacking we got a hexagonal crystal was in in a sense not a surprise we started with 2-dimensional hexagonal layer and we got a 3-dimensional hexagonal crystal.

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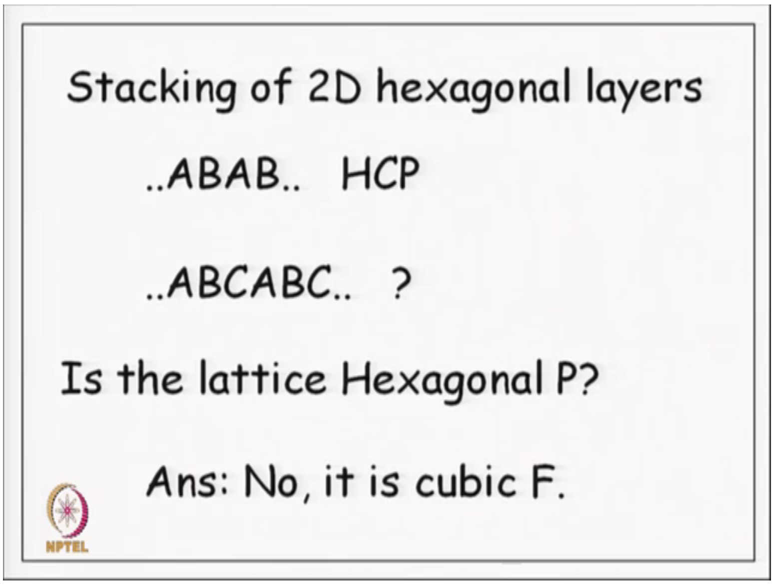

So, ABAB stacking gave us the hexagonal close packed crystal structure. Of course, in terms of lattice we found that the lattices simple hexagonal because there is no lattice like hexagonal close packed. Now we focus on ABC ABC this is our current concern ABC ABC stacking what is the lattice or what is the crystal structure of this ABC ABC stacking. The layers note that the layers are still 2-dimensional hexagonal layer.

So, is the lattice hexagonal P again, but there is a difficulty here because now all since all atoms are equivalent the next layer is also the if we start with an a layer the next layer B is also a lattice point, but this is not exactly above A. So, in a simple hexagonal lattice with one atom motif the next layer should be exactly about bottom layer. This is not true for ABC ABC stacking; obviously, So, the lattice cannot be hexagonal P.

So, the answer and I will say that it is a surprise answer to this question is that the lattice turns out to be cubic F the face centered cubic lattice. I say a surprise answer because our stacking C is the layers which we are stacking a 2-dimensional hexagonal layer. So, the inherent symmetry of the layer is 6-fold symmetry and by stacking them now we are claiming that the crystal structure which we get is face centered cubic.

Face centered cubic structure does not will not have any 6-fold symmetry, our starting 2 d layer was having the 6-fold symmetry. So, where is the 6-fold symmetry lost? Also, the cubic f or face centered cubic will have 4fold axes this is not there in our 2-dimensional hexagonal layer. So, where is this 4fold axis emerging from? So, that is why it is in a way it is rather surprising that by stacking 2-dimensional hexagonal layer we are ending up in a face centered cubic structure which has face centered cubic lattice.

It is not easy to see this in lecture or slides one has to look up models of these structure, but I will try my best to do here and we will do it in reverse let us initially begin with the FCC lattice.

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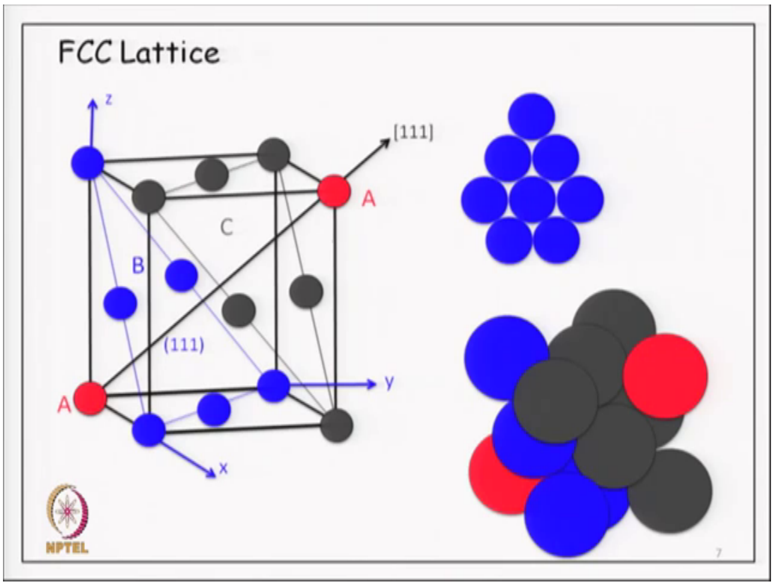

So, for the moment we are forgetting our ABC ABC stacking sequence and we begin with our familiar face centered cubic lattice. So, this is the unit cell of the face centered cubic lattice with lattice point shown as little crosses lattice points are at the corners of the cubic unit cell and at the centers of the faces.

Now, I want to populate this lattice with atoms to get my crystal. So, I want to assign with each lattice point an atom or a group of atoms that is my motif at each lattice point. We have already seen that the structure which we are trying to analyze ABCABC has a single atom motif. So, let us place a single atom that each of these lattice points to I can of course, place atoms at each of these lattice points shown here, but we will do it in sequence or in stages.

So, let us first identify a 1 1 1 plane of this structure to do this we have to first of course, assign the axes. So, let us say these this is our crystallographic axis parallel to the edges of the cube x y and z then a 1 1 1 plane will be and a plane which cuts x y and z at one step or a step of a that is along the corners here. So, this is my 1 1 1 plane identified here with this thin lines.

Now, I place in a in a first step I place atoms only on this plane and one at each lattice point. So, I begin with that corner then I place on this face center and another corner atom bottom face center and that corner there then back face center. So, these are the 6 atoms which are lying on this 1 1 1 plane within the unit cell note notice that 1 1 1 plane will extend in the crystal structure. So, what we are seeing here in this form of this triangle is the intersection of the 1 1 1 plane with the unit cell.

Also notice that this triangle although it not obvious in this perspective diagram, but this triangle is an equilateral triangle because all sides of this triangle are face diagonals of the cube and all face diagonals will be equal they will have a length root 2 times the edge length. So, this is a equilateral triangle and we are placing atoms at the corners and at the midpoints of the sides of that equilateral triangle.

Also notice that the closest distance of approach with between the atoms is along the edges. So, these 2 atoms the corner atom and the face centered atom are the closest atom. So, if we let these atoms grow. So, that they touch along this closest direction then we will have an atom of the size exactly half the diameter of such atoms will be exactly half the face diagonal of the cube.

So, if we place such atoms half the face diagonal diameter half the face diagonal of the cube at all of these sides then we will get a stacking of atoms shown here. So, you can see these 3 atoms one 2 and 3 let us say representing this one 2 and 3 the left face diagonal of the cube, but they are touching here it is there for clarity I have not shown them touching here now I am emphasizing that actually these atoms can be touching.

So, these are the 3 atoms on the left face diagonal and these 3 atoms on the bottom face diagonal and these 3 atoms on the back-face diagonal. So, I get a triangular arrangement of atoms like this, but if you now look at it carefully you will realize that this is nothing but a piece of a close packed plane the 2 dimensional hexagonal close packed plane which we were considering where each atom is surrounded by 6 atom not immediately obvious in this triangle, but notice that the plane will extend and there will be more atoms added to this in the real crystal and if I add 2 atoms to bring out the hexagon you can see that this central atom is in contact with 6 atom.

So, this piece what I am trying to show that this piece of 1 1 1 plane within the unit cell is actually a part of a close packed plane in the structure. So, the 1 1 1 plane in an FCC lattice becomes a close packed a close packed plane let us look at let us look at the other plane parallel to this close packed plane. So, I have another triangle here these 6 atoms are also forming a plane which is exactly parallel to this plane and if I place atoms on these also then I have a next layer of close packed plane about this.

Also notice that the 1 1 1 planes in a cubic crystal are perpendicular to the 1 1 one direction and the 1 1 one direction is the body diagonal which means the planes which we are considering these 1 1 1 planes are planes perpendicular to A Body diagonal of the cube. So, our conclusion is that planes perpendicular to the body diagonals of the cube are close packed plane.

But what is their stacking sequence. So, we now place 2 more atoms at the endpoints of this body diagonal and I show them in red. So, if you now carefully observe and this is where a model is very, very essential, but you can try your imagination to it is best capability here that if we now look at this red atom if this is also not a single atom in the structure in this unit cell it is a single atom, but in the structure this is a representative again of another close packed plane similar to this blue layer or the black layer passing through this corner.

So, I have close packed plane at this red level then the blue level and then the black level and again at the red level and if you observe there a stacking sequence then if I call this red layer a then the blue layer is B the black layer is C and then again on the body diagonal we have e. So, the stacking sequence of these close packed layers is exactly what we were looking for ABC ABC.

So, what we conclude here from this analysis that planes perpendicular to the body diagonal in an FCC lattice form a closed pack 2 dimensional hexagonal close packed layers if they are populated if the lattice points if at the lattice points we place atoms of the right size and by right size we mean diameter equal to half the face diagonal. So, if we do this then we convert the FCC lattice into a structure in which can be thought of as stacking of close packed layers in a sequence ABC ABC this is more clearly seen in this diagram where now the atoms are actually shown touching for to bring out the fact that the in the close pack layer atoms are touching.

So, such models can easily be made by balls and you can try that at home. So, let us come back we.

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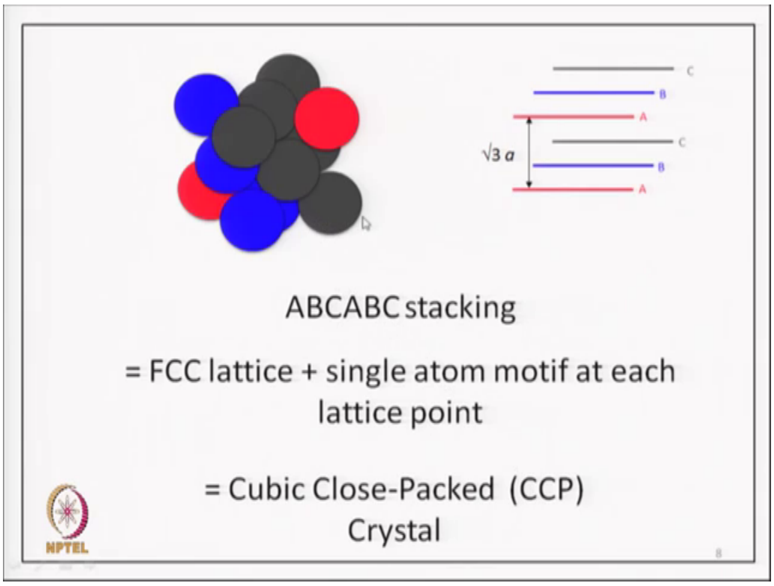

Have now analyzed both the lattice and motif; so we summarize our results that the ABC ABC stacking is nothing but a stacking of close packed planes in the ABC ABC sequence and these can be thought of as planes perpendicular to the body diagonal of the cube which is our unit cell. So, a cubic unit cell can be identified whose body diagonal is perpendicular to the plane stacking planes or the 2 dimensional hexagonal planes which we are stacking.

So, the lattice becomes face centered cubic and the motif as we have already analyzed is a single atom motif at each lattice point. So, this completes our analysis in terms of lattice and motif, but the we just add one more point the crystal structure the name of the crystal structure and appropriate name of the crystal structure should be cubic close packed CCP to contrast it with the hexagonal close packed h cp which we have already used.

But for some region CCP is not very common in literature and this kind of a structure is often called an FCC crystal; however, we are trying to make by calling it the cubic close packed crystal we are trying to make a distinction between the crystal and the lattice. So, the crystal is cubic close packed and it has a lattice which is FCC and has a motif which is one atom at each lattice point. So, let us now let us now look at some interesting examples not from crystal.

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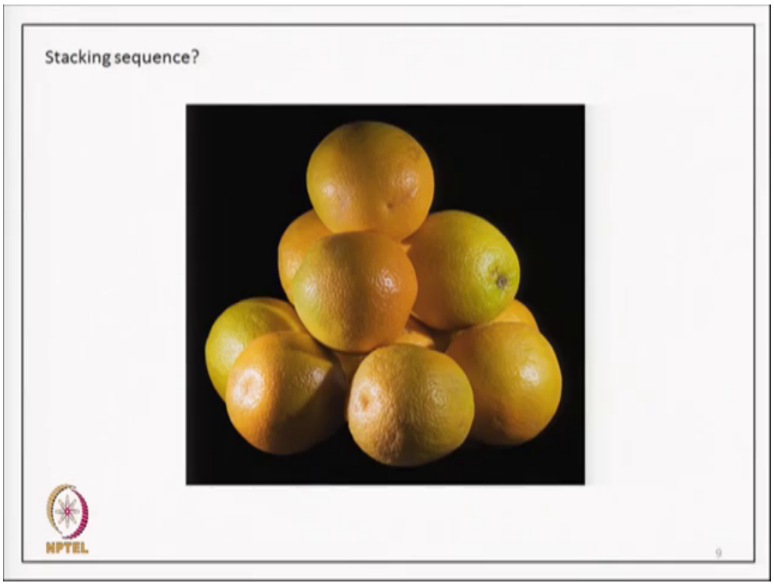

But from our normal life experience here is fruit the oranges is stacked on in a fruit seller shop.

So, the oranges are approximate it spheres and you can see that they are stacked one above the other and I leave this question to you that what is the stacking sequence what is the stacking sequence in which these oranges are stacked is it A B A B or is it ABC ABC that is it hexagonal close pack or is it cubic close packed.

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Another yummy example from a sweet shop from fruit seller shop we now go to the sweet shop and here ladoos yummy ladoos are stacked one above the other again the question what is the stacking sequence and I end.

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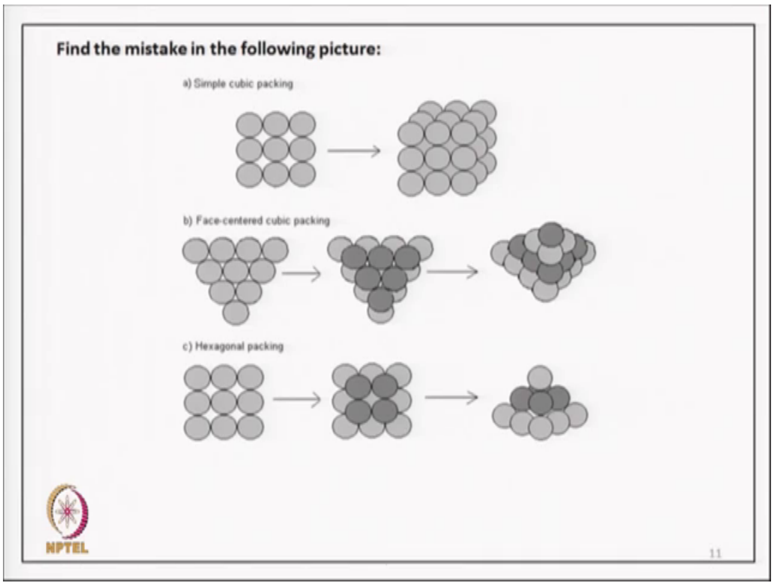

This video with a slide which shows the picture available on the web and it is showing simple cubic packing face centered cubic packing and hexagonal packing, but there is a mistake in this picture and if you have understood the lecture till now about the cubic about the packing of closed pack layers you should be able to identify what is the mistake in the spectrum.

So, with this I end this video and we will meet again.